



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 02:58 pm BST

PDB ID : 3C0Z
Title : Crystal structure of catalytic domain of human histone deacetylase HDAC7 in complex with SAHA
Authors : Min, J.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2008-01-21
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

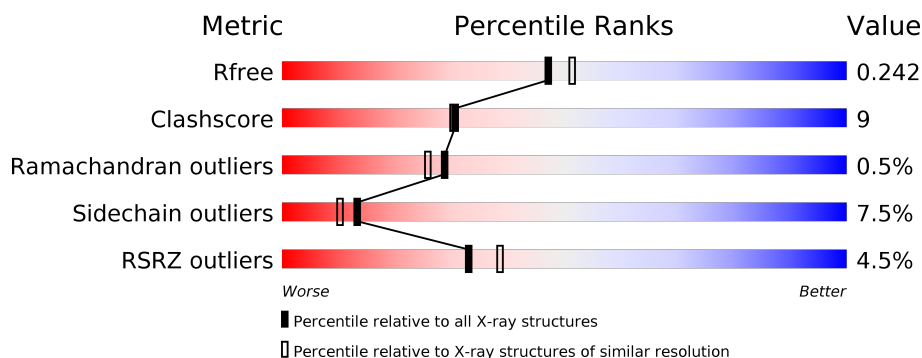
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	B	423	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>• 13%</div> </div> </div>
1	C	423	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>• 15%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8769 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone deacetylase 7a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2885	1810	516	540	19			
1	B	368	Total	C	N	O	S	0	0	0
			2791	1748	506	518	19			
1	C	359	Total	C	N	O	S	0	0	0
			2724	1703	493	510	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4
B	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4
C	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

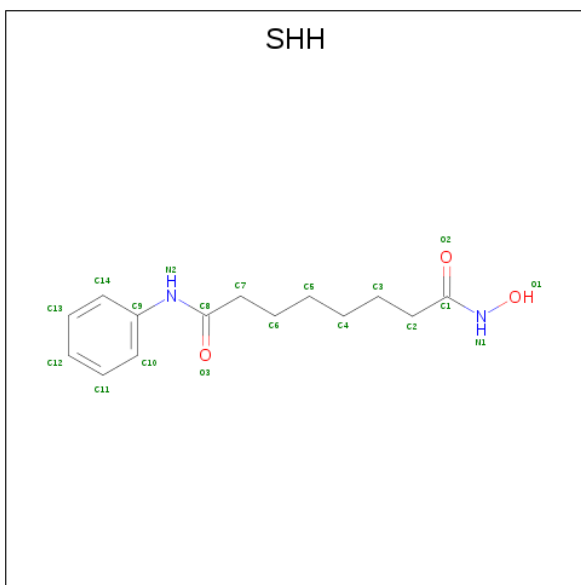
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total K 2 2	0	0

- Molecule 4 is OCTANEDIOIC ACID HYDROXYAMIDE PHENYLAMIDE (three-letter code: SHH) (formula: $C_{14}H_{20}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 5 1 2	0	0
4	B	1	Total C N O 9 6 1 2	0	0
4	C	1	Total C N O 8 5 1 2	0	0

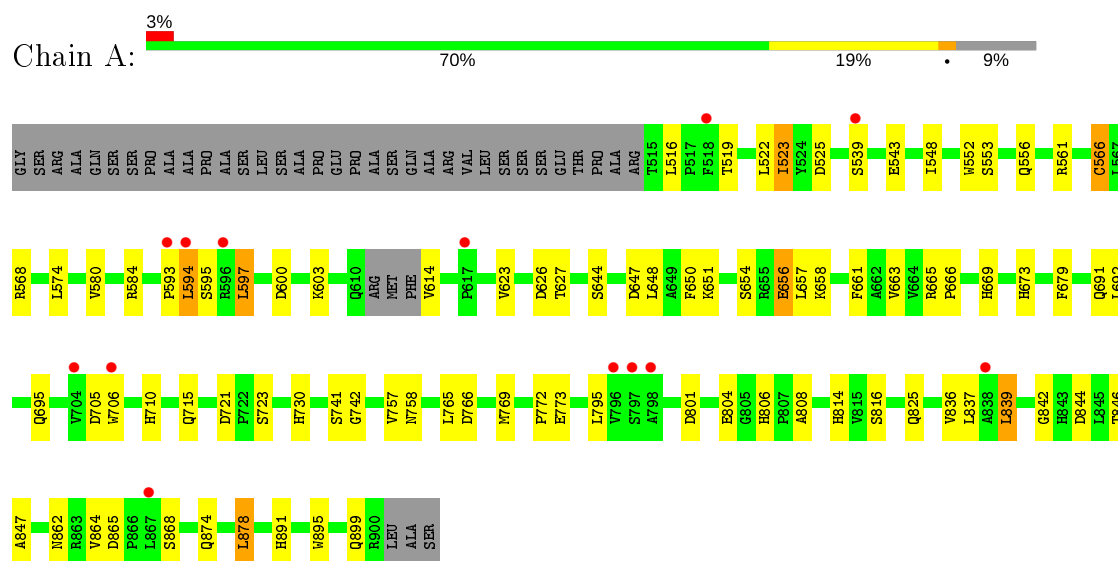
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	127	Total O 127 127	0	0
5	B	111	Total O 111 111	0	0
5	C	94	Total O 94 94	0	0

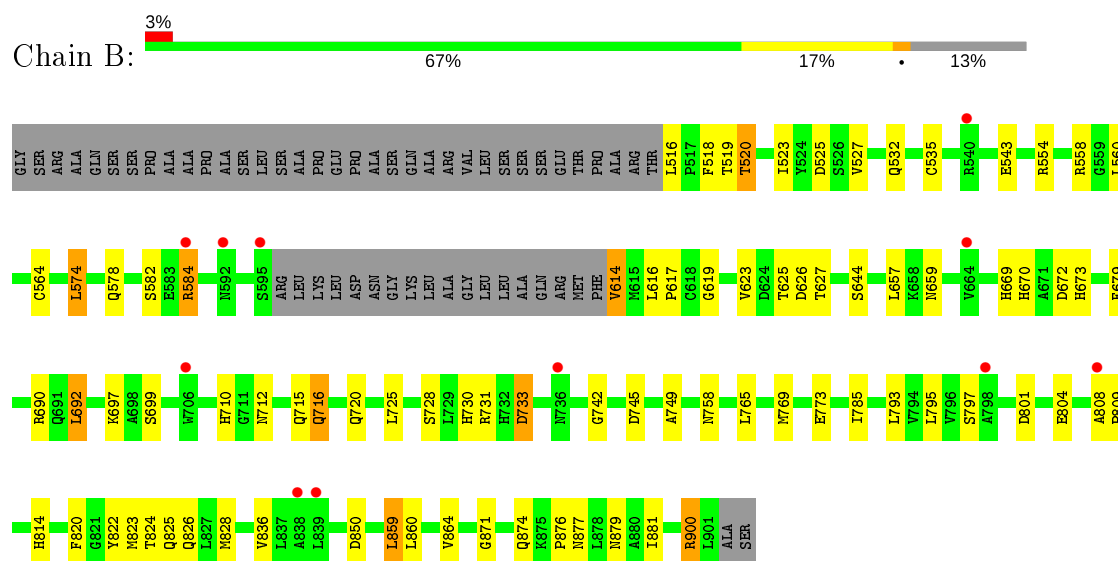
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

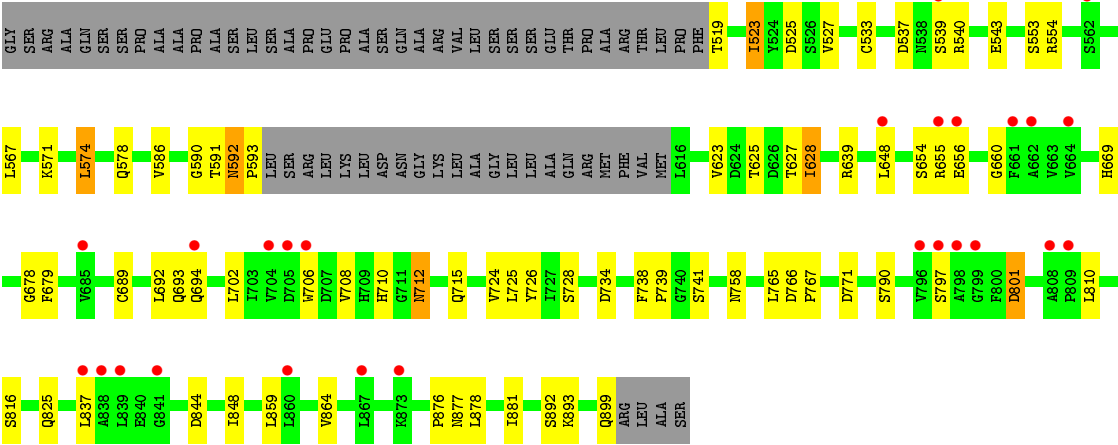
- Molecule 1: Histone deacetylase 7a



- Molecule 1: Histone deacetylase 7a



- Molecule 1: Histone deacetylase 7a



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.83Å 81.83Å 148.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.10 32.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (40.00-2.10) 93.4 (32.95-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.243 0.194 , 0.242	Depositor DCC
R_{free} test set	3080 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l 0.031 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8769	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SHH, ZN, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	1/2953 (0.0%)	0.83	1/4010 (0.0%)
1	B	0.90	1/2859 (0.0%)	0.87	3/3879 (0.1%)
1	C	0.76	0/2790	0.78	0/3787
All	All	0.84	2/8602 (0.0%)	0.83	4/11676 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	CYS	CB-SG	-5.66	1.72	1.81
1	A	566	CYS	CB-SG	-5.36	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	690	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	692	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	900	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	705	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2885	0	2765	58	0
1	B	2791	0	2679	51	0
1	C	2724	0	2606	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	0
4	A	8	0	7	0	0
4	B	9	0	9	1	0
4	C	8	0	7	0	0
5	A	127	0	0	6	0
5	B	111	0	0	6	0
5	C	94	0	0	2	0
All	All	8769	0	8073	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ASP:OD2	1:C:527:VAL:HG23	1.40	1.22
1:A:650:PHE:HE2	1:A:695:GLN:HG2	1.25	0.98
1:A:650:PHE:CE2	1:A:695:GLN:HG2	2.04	0.92
1:B:623:VAL:HG22	1:B:627:THR:HB	1.55	0.87
1:A:566:CYS:SG	5:A:997:HOH:O	2.03	0.86
1:A:519:THR:O	1:A:658:LYS:N	2.09	0.85
1:A:523:ILE:HG21	1:A:644:SER:HB3	1.59	0.84
1:B:672:ASP:HB2	1:B:716:GLN:HE21	1.44	0.83
1:A:825:GLN:HE22	1:A:864:VAL:H	1.22	0.82
1:B:614:VAL:N	5:B:1009:HOH:O	2.15	0.80
1:B:769:MET:CE	5:B:945:HOH:O	2.27	0.80
1:C:525:ASP:OD2	1:C:527:VAL:CG2	2.29	0.75
1:C:825:GLN:HE22	1:C:864:VAL:H	1.33	0.74
1:C:592:ASN:HB2	1:C:593:PRO:HA	1.71	0.72
1:A:556:GLN:HB2	1:A:561:ARG:NE	2.04	0.71
1:C:892:SER:O	1:C:899:GLN:CG	2.38	0.71
1:A:825:GLN:NE2	1:A:864:VAL:H	1.87	0.70
1:A:804:GLU:OE1	1:A:814:HIS:HD2	1.74	0.70
1:B:733:ASP:OD1	5:B:982:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ARG:NH2	1:B:850:ASP:OD1	2.22	0.69
1:B:525:ASP:OD2	1:B:527:VAL:HG23	1.92	0.69
1:C:715:GLN:HE22	1:C:758:ASN:HD21	1.39	0.69
1:A:650:PHE:HE2	1:A:695:GLN:CG	2.05	0.68
1:B:876:PRO:HG2	1:B:881:ILE:HD11	1.74	0.68
1:C:712:ASN:H	1:C:712:ASN:HD22	1.43	0.67
1:B:715:GLN:HE22	1:B:758:ASN:HD21	1.42	0.67
1:A:651:LYS:HB3	1:A:657:LEU:HD12	1.76	0.67
1:B:520:THR:HB	1:B:659:ASN:OD1	1.95	0.67
1:C:825:GLN:NE2	1:C:864:VAL:H	1.91	0.67
1:A:715:GLN:HE22	1:A:758:ASN:HD21	1.41	0.66
1:C:892:SER:O	1:C:899:GLN:HG3	1.95	0.65
1:B:769:MET:HE1	5:B:945:HOH:O	1.91	0.65
3:C:202:K:K	5:C:905:HOH:O	2.08	0.64
1:A:626:ASP:HB3	1:A:679:PHE:CE1	2.33	0.63
1:B:673:HIS:H	1:B:716:GLN:HE22	1.43	0.63
1:A:661:PHE:CE1	1:A:663:VAL:HG22	2.33	0.62
1:B:824:THR:O	1:B:828:MET:HG3	2.01	0.60
1:A:721:ASP:OD1	1:A:723:SER:OG	2.16	0.59
1:A:804:GLU:OE1	1:A:814:HIS:CD2	2.53	0.59
1:B:670:HIS:HD1	1:B:712:ASN:ND2	2.00	0.59
1:A:862:ASN:HB2	5:A:994:HOH:O	2.03	0.58
1:B:673:HIS:H	1:B:716:GLN:NE2	2.01	0.58
1:B:584:ARG:H	1:B:584:ARG:HD3	1.67	0.58
1:B:574:LEU:O	1:B:578:GLN:HG3	2.04	0.58
1:C:702:LEU:HD13	1:C:725:LEU:HD23	1.85	0.58
1:C:623:VAL:HG22	1:C:627:THR:HB	1.86	0.58
1:B:825:GLN:HE22	1:B:864:VAL:H	1.51	0.57
1:A:556:GLN:HB2	1:A:561:ARG:CZ	2.35	0.57
1:C:523:ILE:HD13	1:C:567:LEU:HB2	1.86	0.57
1:C:876:PRO:HG2	1:C:881:ILE:HD11	1.87	0.57
1:B:626:ASP:HB3	1:B:679:PHE:CE1	2.40	0.56
1:A:595:SER:HB3	1:A:597:LEU:HB2	1.87	0.56
1:B:623:VAL:CG2	1:B:627:THR:HB	2.31	0.56
1:B:670:HIS:NE2	4:B:301:SHH:N1	2.54	0.56
1:B:715:GLN:NE2	1:B:758:ASN:HD21	2.03	0.56
1:A:661:PHE:HD2	1:A:837:LEU:HB2	1.70	0.55
1:B:523:ILE:HG21	1:B:644:SER:HB3	1.89	0.55
1:B:769:MET:SD	1:B:773:GLU:HG2	2.47	0.55
1:A:523:ILE:HG13	1:A:648:LEU:HB2	1.89	0.54
1:C:892:SER:O	1:C:899:GLN:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:SER:HB3	5:A:993:HOH:O	2.08	0.54
1:A:626:ASP:HB3	1:A:679:PHE:HE1	1.74	0.53
1:A:710:HIS:HD2	1:A:741:SER:OG	1.91	0.53
1:C:586:VAL:O	1:C:590:GLY:N	2.41	0.53
1:C:592:ASN:CB	1:C:593:PRO:HA	2.39	0.53
1:C:710:HIS:HD2	1:C:741:SER:OG	1.92	0.53
1:A:651:LYS:CB	1:A:657:LEU:HD12	2.38	0.53
1:B:814:HIS:CD2	5:B:951:HOH:O	2.62	0.53
1:A:584:ARG:HD3	5:A:1023:HOH:O	2.08	0.53
1:C:537:ASP:OD2	1:C:540:ARG:HG2	2.07	0.53
1:C:715:GLN:NE2	1:C:758:ASN:HD21	2.06	0.52
1:A:654:SER:O	1:C:571:LYS:HE3	2.10	0.52
1:A:730:HIS:HE1	1:A:742:GLY:O	1.93	0.52
1:A:656:GLU:HG2	1:C:591:THR:HB	1.92	0.51
1:C:574:LEU:HD13	1:C:639:ARG:NH1	2.25	0.51
1:A:795:LEU:HD23	1:A:836:VAL:HB	1.91	0.50
1:C:726:TYR:CZ	1:C:728:SER:HB2	2.47	0.50
1:A:650:PHE:HE1	1:A:691:GLN:HB3	1.75	0.49
1:B:730:HIS:HE1	1:B:742:GLY:O	1.95	0.49
1:A:710:HIS:CE1	1:A:715:GLN:NE2	2.81	0.49
1:C:771:ASP:OD2	1:C:816:SER:HB3	2.13	0.49
1:B:877:ASN:OD1	1:B:879:ASN:HB2	2.13	0.49
1:C:586:VAL:O	1:C:590:GLY:HA3	2.12	0.49
1:C:693:GLN:HE22	1:C:724:VAL:HG23	1.79	0.47
1:B:804:GLU:OE1	1:B:814:HIS:ND1	2.37	0.47
1:A:580:VAL:O	1:A:673:HIS:HD2	1.97	0.47
1:A:650:PHE:CE1	1:A:691:GLN:HB3	2.49	0.47
1:A:825:GLN:NE2	1:A:864:VAL:HG23	2.30	0.47
1:B:712:ASN:H	1:B:712:ASN:HD22	1.61	0.46
1:A:523:ILE:HG21	1:A:644:SER:CB	2.40	0.46
1:C:678:GLY:O	1:C:679:PHE:HB2	2.15	0.46
1:C:533:CYS:HB2	1:C:628:ILE:HG13	1.97	0.46
1:B:822:TYR:O	1:B:826:GLN:HG3	2.15	0.46
1:B:871:GLY:HA2	1:B:874:GLN:HG2	1.97	0.46
1:C:766:ASP:HA	1:C:767:PRO:C	2.36	0.46
1:A:844:ASP:HB3	1:A:847:ALA:HB3	1.97	0.46
1:A:665:ARG:HB2	1:A:666:PRO:HA	1.98	0.46
1:C:712:ASN:H	1:C:712:ASN:ND2	2.11	0.45
1:B:725:LEU:HD21	1:B:785:ILE:HG22	1.98	0.45
1:C:689:CYS:O	1:C:693:GLN:HG3	2.17	0.45
1:A:730:HIS:CE1	1:A:742:GLY:O	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:THR:HG23	1:B:860:LEU:HD23	1.98	0.45
1:A:895:TRP:O	1:A:899:GLN:HG3	2.16	0.45
1:B:824:THR:CG2	1:B:859:LEU:HD13	2.47	0.45
1:B:672:ASP:HB2	1:B:716:GLN:NE2	2.23	0.44
1:C:648:LEU:HD11	1:C:660:GLY:HA3	1.98	0.44
1:A:553:SER:HA	1:A:561:ARG:HH11	1.81	0.44
1:A:595:SER:C	1:A:597:LEU:H	2.20	0.44
1:A:595:SER:HB3	1:A:597:LEU:H	1.83	0.44
1:C:844:ASP:O	1:C:848:ILE:HG23	2.17	0.44
1:A:600:ASP:OD2	1:A:603:LYS:HG2	2.17	0.44
1:B:795:LEU:HD23	1:B:836:VAL:HB	1.99	0.44
1:B:582:SER:HB3	1:B:673:HIS:CE1	2.52	0.44
1:B:730:HIS:CE1	1:B:742:GLY:O	2.71	0.44
1:A:522:LEU:HD23	1:A:661:PHE:HB3	2.01	0.43
1:A:548:ILE:HG22	1:A:839:LEU:HD12	2.01	0.43
1:C:801:ASP:OD1	1:C:801:ASP:N	2.32	0.43
1:A:757:VAL:HG22	1:A:891:HIS:CE1	2.53	0.43
1:A:865:ASP:HB3	1:A:868:SER:HB3	2.00	0.43
1:A:593:PRO:HA	1:A:594:LEU:HA	1.68	0.43
1:A:772:PRO:HD2	1:A:773:GLU:OE1	2.18	0.43
1:C:654:SER:C	1:C:656:GLU:H	2.21	0.43
1:B:584:ARG:H	1:B:584:ARG:CD	2.29	0.42
1:B:560:LEU:HA	1:B:560:LEU:HD23	1.71	0.42
1:B:728:SER:OG	1:B:730:HIS:HD2	2.02	0.42
1:C:693:GLN:NE2	1:C:724:VAL:CG2	2.82	0.42
1:A:552:TRP:CE3	1:A:552:TRP:HA	2.54	0.42
1:C:767:PRO:HG2	1:C:877:ASN:HB2	2.00	0.42
1:A:650:PHE:CE2	1:A:695:GLN:CG	2.89	0.42
1:A:525:ASP:OD1	1:A:568:ARG:HD2	2.19	0.42
1:B:616:LEU:O	1:B:619:GLY:N	2.37	0.42
1:C:710:HIS:HE1	1:C:715:GLN:NE2	2.17	0.42
1:A:878:LEU:HA	1:A:878:LEU:HD13	1.89	0.42
1:A:801:ASP:HB3	1:A:842:GLY:HA2	2.01	0.41
1:B:697:LYS:HA	1:B:697:LYS:HD2	1.88	0.41
1:B:710:HIS:CE1	1:B:715:GLN:NE2	2.88	0.41
1:C:693:GLN:HE22	1:C:724:VAL:CG2	2.33	0.41
1:C:837:LEU:N	1:C:837:LEU:HD23	2.34	0.41
1:C:893:LYS:NZ	5:C:987:HOH:O	2.52	0.41
1:A:623:VAL:HG22	1:A:627:THR:HB	2.03	0.41
1:A:806:HIS:O	5:A:1009:HOH:O	2.22	0.41
1:C:710:HIS:CE1	1:C:715:GLN:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:PHE:HA	1:C:739:PRO:HA	1.87	0.41
1:C:586:VAL:O	1:C:590:GLY:CA	2.67	0.41
1:B:825:GLN:HG3	5:B:926:HOH:O	2.21	0.40
1:B:720:GLN:HA	1:B:749:ALA:O	2.21	0.40
1:B:731:ARG:CZ	1:B:765:LEU:HD21	2.51	0.40
1:B:820:PHE:HA	1:B:823:MET:HE2	2.03	0.40
1:A:519:THR:N	5:A:962:HOH:O	2.55	0.40
1:B:554:ARG:HD2	1:B:558:ARG:HG3	2.04	0.40
1:B:808:ALA:HA	1:B:809:PRO:HA	1.91	0.40
1:B:879:ASN:HA	1:B:879:ASN:HD22	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/423 (90%)	364 (96%)	14 (4%)	1 (0%)	41	41
1	B	364/423 (86%)	343 (94%)	18 (5%)	3 (1%)	19	15
1	C	355/423 (84%)	338 (95%)	16 (4%)	1 (0%)	41	41
All	All	1098/1269 (86%)	1045 (95%)	48 (4%)	5 (0%)	29	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	PHE
1	A	808	ALA
1	C	592	ASN
1	B	733	ASP
1	B	617	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/336 (89%)	280 (93%)	20 (7%)	16	13
1	B	292/336 (87%)	271 (93%)	21 (7%)	14	11
1	C	285/336 (85%)	260 (91%)	25 (9%)	10	6
All	All	877/1008 (87%)	811 (92%)	66 (8%)	13	10

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	516	LEU
1	A	523	ILE
1	A	539	SER
1	A	543	GLU
1	A	574	LEU
1	A	594	LEU
1	A	597	LEU
1	A	614	VAL
1	A	647	ASP
1	A	656	GLU
1	A	669	HIS
1	A	692	LEU
1	A	706	TRP
1	A	765	LEU
1	A	766	ASP
1	A	769	MET
1	A	839	LEU
1	A	846	THR
1	A	874	GLN
1	A	878	LEU
1	B	516	LEU
1	B	519	THR
1	B	520	THR
1	B	532	GLN
1	B	535	CYS
1	B	543	GLU

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Mol	Chain	Res	Type
1	B	574	LEU
1	B	584	ARG
1	B	614	VAL
1	B	625	THR
1	B	657	LEU
1	B	669	HIS
1	B	692	LEU
1	B	699	SER
1	B	716	GLN
1	B	745	ASP
1	B	793	LEU
1	B	797	SER
1	B	801	ASP
1	B	859	LEU
1	B	900	ARG
1	C	519	THR
1	C	523	ILE
1	C	539	SER
1	C	543	GLU
1	C	553	SER
1	C	554	ARG
1	C	574	LEU
1	C	578	GLN
1	C	625	THR
1	C	628	ILE
1	C	655	ARG
1	C	669	HIS
1	C	692	LEU
1	C	694	GLN
1	C	706	TRP
1	C	708	VAL
1	C	712	ASN
1	C	734	ASP
1	C	765	LEU
1	C	790	SER
1	C	797	SER
1	C	801	ASP
1	C	810	LEU
1	C	859	LEU
1	C	878	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	GLN
1	A	673	HIS
1	A	710	HIS
1	A	712	ASN
1	A	715	GLN
1	A	716	GLN
1	A	730	HIS
1	A	756	ASN
1	A	814	HIS
1	A	825	GLN
1	A	899	GLN
1	B	532	GLN
1	B	636	ASN
1	B	673	HIS
1	B	710	HIS
1	B	712	ASN
1	B	715	GLN
1	B	716	GLN
1	B	730	HIS
1	B	756	ASN
1	B	825	GLN
1	B	862	ASN
1	B	879	ASN
1	B	899	GLN
1	C	673	HIS
1	C	693	GLN
1	C	710	HIS
1	C	712	ASN
1	C	715	GLN
1	C	730	HIS
1	C	756	ASN
1	C	825	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SHH	A	301	2	7,7,19	0.53	0	6,7,22	1.58	1 (16%)
4	SHH	C	301	2	7,7,19	0.86	0	6,7,22	0.51	0
4	SHH	B	301	2	8,8,19	1.27	1 (12%)	7,8,22	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SHH	A	301	2	-	2/6/6/15	-
4	SHH	C	301	2	-	2/6/6/15	-
4	SHH	B	301	2	-	3/7/7/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	SHH	C1-N1	2.94	1.35	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	SHH	O2-C1-N1	-3.70	118.72	123.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

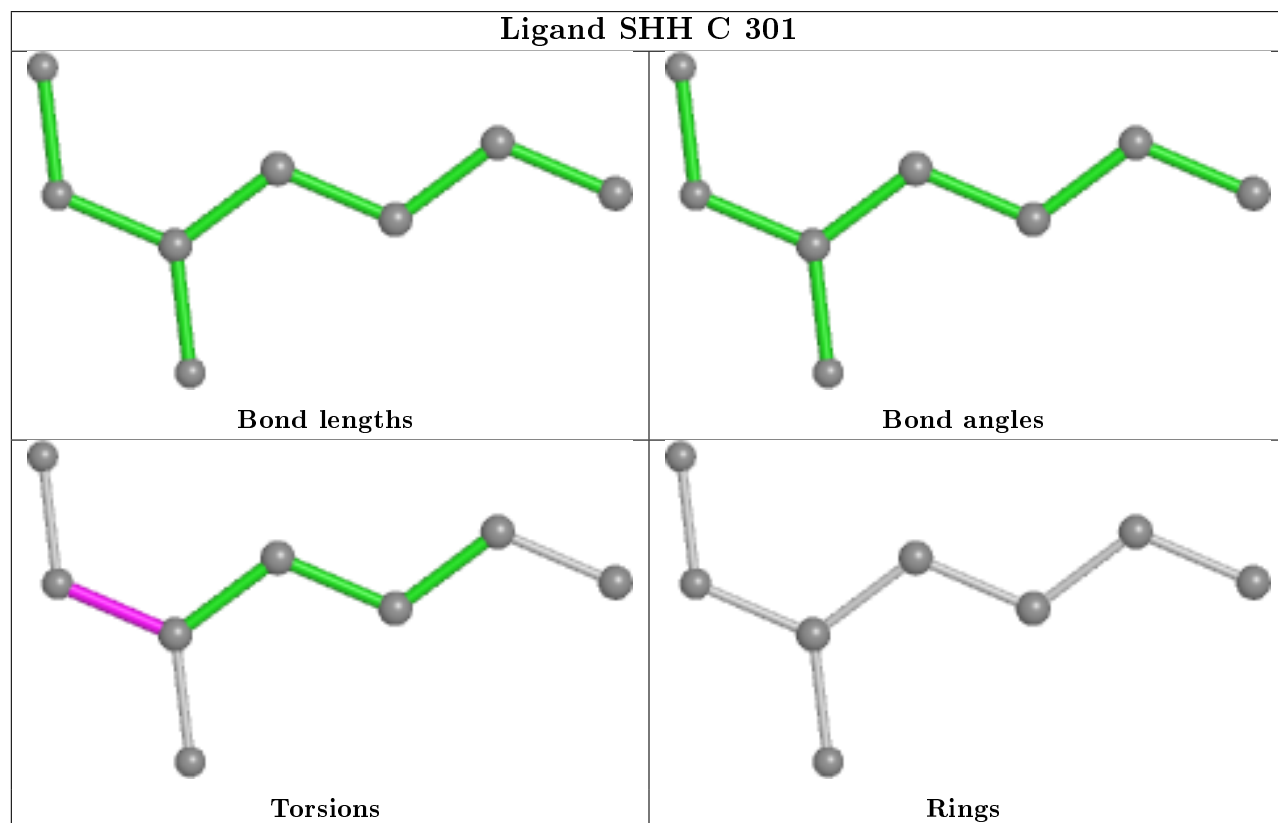
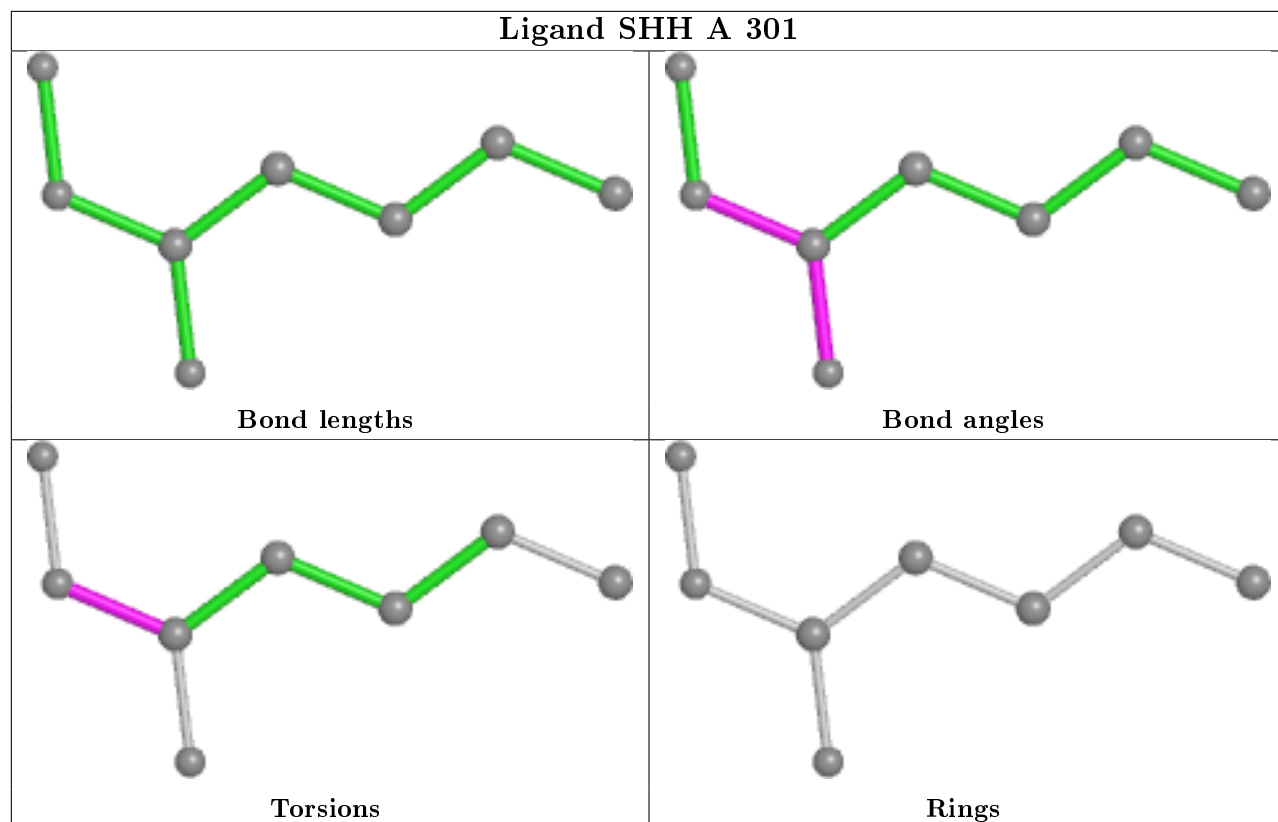
Mol	Chain	Res	Type	Atoms
4	C	301	SHH	O2-C1-N1-O1
4	C	301	SHH	C2-C1-N1-O1
4	B	301	SHH	O2-C1-N1-O1
4	B	301	SHH	C2-C1-N1-O1
4	A	301	SHH	O2-C1-N1-O1
4	A	301	SHH	C2-C1-N1-O1
4	B	301	SHH	C2-C3-C4-C5

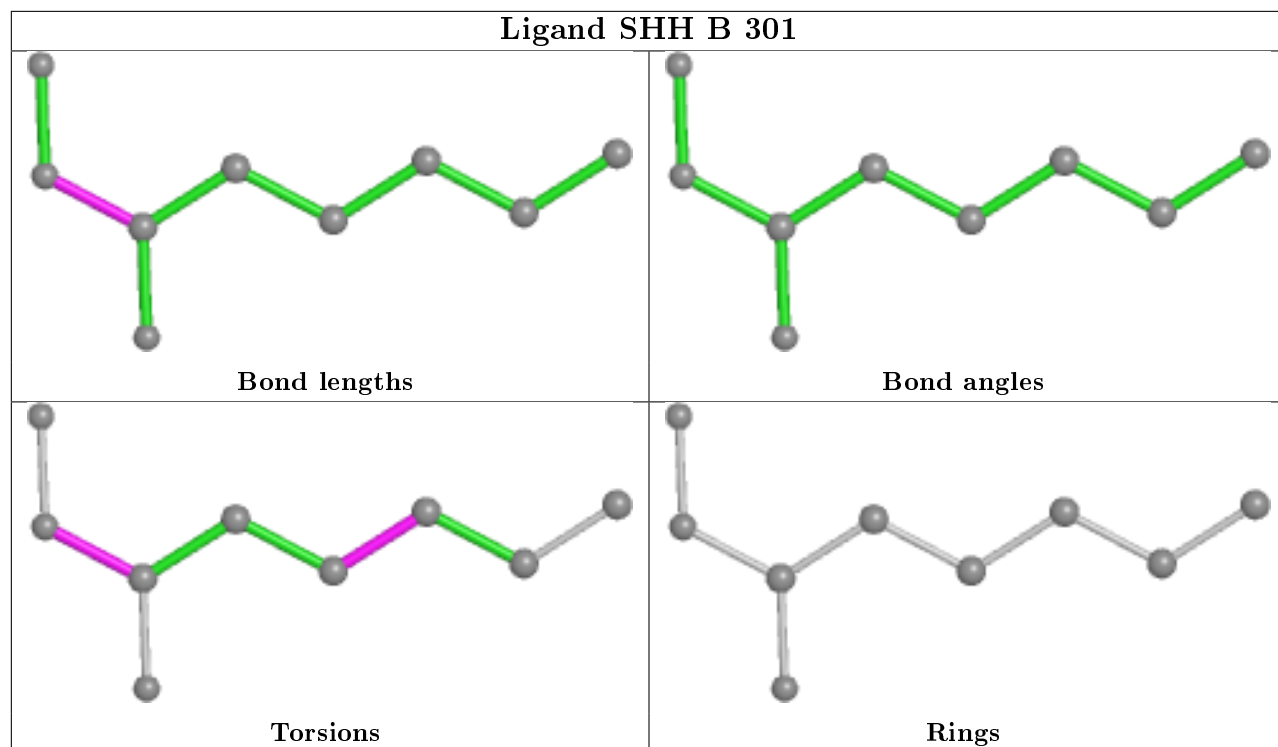
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	SHH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/423 (90%)	0.06	13 (3%) 45 51	19, 34, 52, 62	0
1	B	368/423 (86%)	-0.00	11 (2%) 50 56	19, 33, 53, 60	0
1	C	359/423 (84%)	0.23	26 (7%) 15 19	25, 41, 60, 66	0
All	All	1110/1269 (87%)	0.09	50 (4%) 33 38	19, 36, 56, 66	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	796	VAL	5.8
1	C	706	TRP	3.8
1	A	518	PHE	3.7
1	A	617	PRO	3.7
1	C	704	VAL	3.7
1	C	837	LEU	3.6
1	C	838	ALA	3.6
1	C	685	VAL	3.4
1	C	797	SER	3.3
1	C	798	ALA	3.2
1	C	808	ALA	3.1
1	A	706	TRP	3.1
1	C	562	SER	3.0
1	C	839	LEU	3.0
1	B	839	LEU	2.8
1	A	704	VAL	2.7
1	A	596	ARG	2.7
1	B	706	TRP	2.7
1	C	809	PRO	2.7
1	B	838	ALA	2.7
1	C	662	ALA	2.6
1	B	592	ASN	2.5
1	C	873	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	655	ARG	2.5
1	A	838	ALA	2.5
1	A	593	PRO	2.5
1	C	661	PHE	2.4
1	A	594	LEU	2.4
1	A	798	ALA	2.3
1	C	799	GLY	2.3
1	C	841	GLY	2.3
1	A	797	SER	2.3
1	B	798	ALA	2.2
1	B	595	SER	2.2
1	B	736	ASN	2.2
1	A	796	VAL	2.2
1	B	540	ARG	2.2
1	C	860	LEU	2.2
1	C	867	LEU	2.1
1	C	705	ASP	2.1
1	A	867	LEU	2.1
1	A	539	SER	2.1
1	C	656	GLU	2.1
1	C	648	LEU	2.1
1	B	664	VAL	2.1
1	C	539	SER	2.0
1	B	808	ALA	2.0
1	B	584	ARG	2.0
1	C	664	VAL	2.0
1	C	694	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

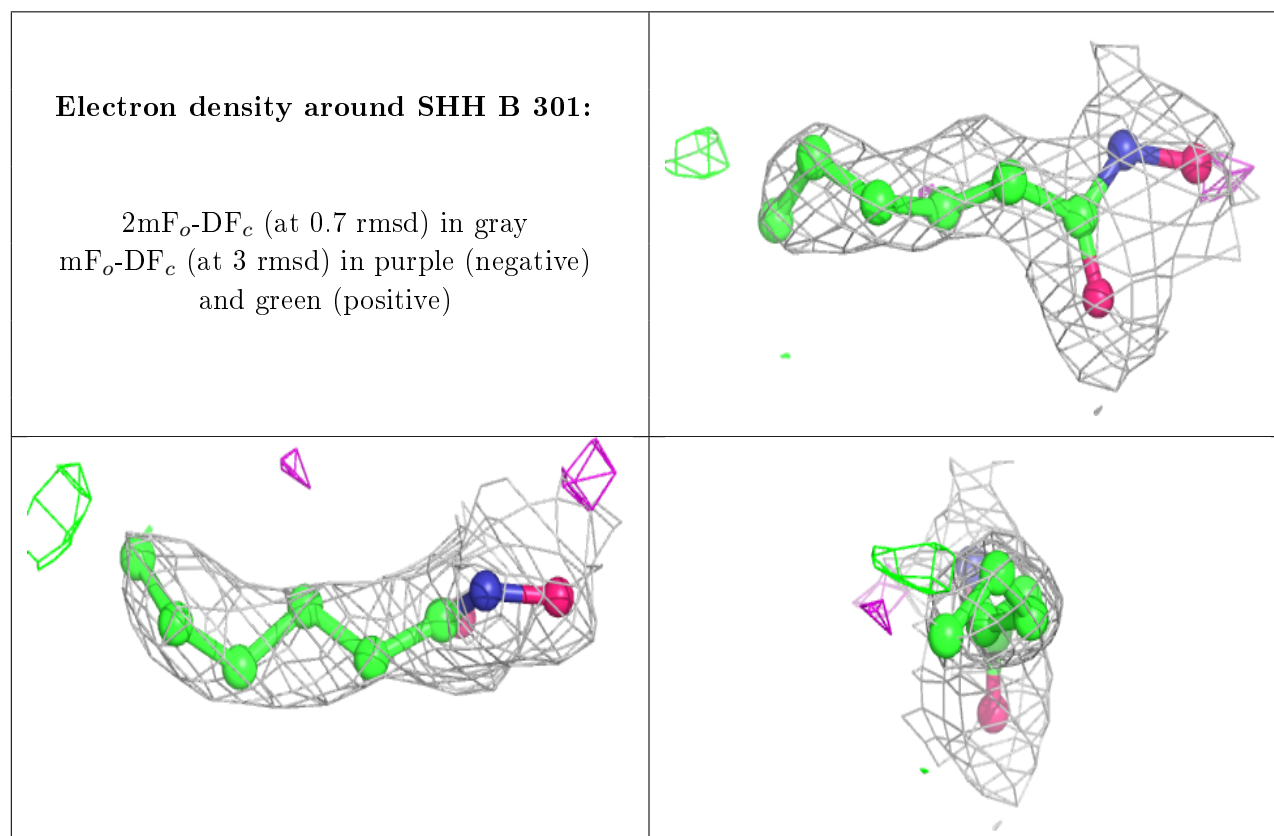
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

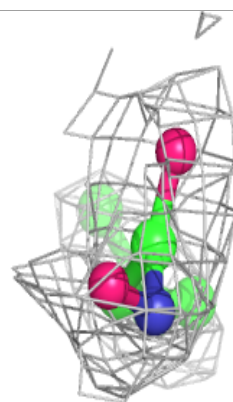
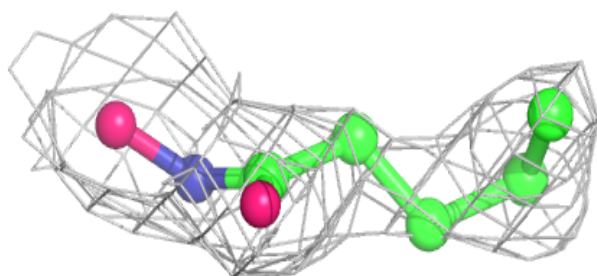
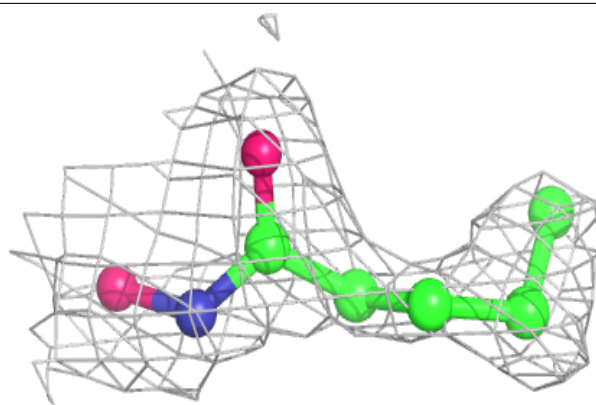
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SHH	B	301	9/19	0.95	0.11	34,40,49,52	0
4	SHH	C	301	8/19	0.96	0.14	34,42,44,44	0
4	SHH	A	301	8/19	0.96	0.14	39,48,49,51	0
3	K	B	202	1/1	0.98	0.16	31,31,31,31	0
3	K	C	201	1/1	0.98	0.04	34,34,34,34	0
3	K	C	202	1/1	0.99	0.08	40,40,40,40	0
2	ZN	A	102	1/1	0.99	0.05	40,40,40,40	0
3	K	A	201	1/1	0.99	0.05	27,27,27,27	0
3	K	B	201	1/1	0.99	0.06	30,30,30,30	0
2	ZN	C	102	1/1	0.99	0.04	50,50,50,50	0
2	ZN	B	101	1/1	0.99	0.06	35,35,35,35	0
3	K	A	202	1/1	0.99	0.05	36,36,36,36	0
2	ZN	A	101	1/1	1.00	0.09	31,31,31,31	0
2	ZN	C	101	1/1	1.00	0.06	36,36,36,36	0
2	ZN	B	102	1/1	1.00	0.04	46,46,46,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

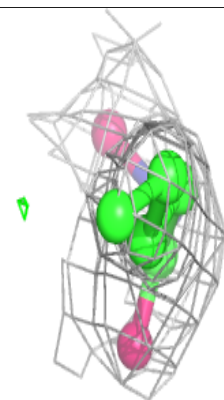
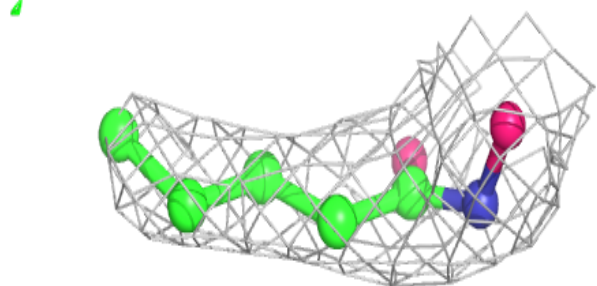
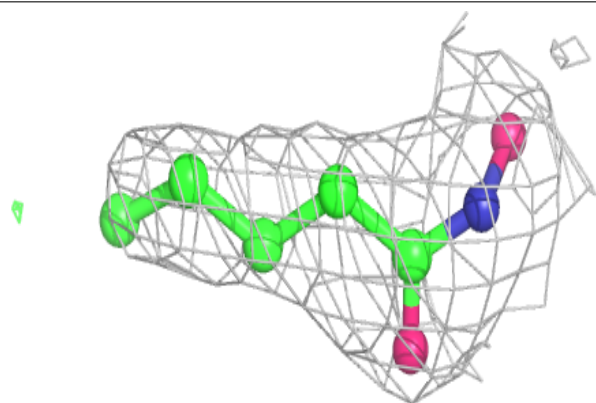


Electron density around SHH C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SHH A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.